Prediction of Thermonuclear Reaction Rates in Astrophysics

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Abstract. Recent improvements and remaining problems in the prediction of thermonuclear rates are reviewed. The main emphasis is on statistical model calculations, but the challenge to include direct reactions close to the driplines is also briefly addressed. Further theoretical as well as experimental investigations are motivated.

1 Introduction

The investigation of explosive nuclear burning in astrophysical environments is a challenge for both theoretical and experimental nuclear physicists. Highly unstable nuclei are produced in such processes which again can be targets for subsequent reactions. Cross sections and astrophysical reaction rates for a large number of nuclei are required to perform complete network calculations which take into account all possible reaction links and do not postulate a priori simplifications. Most of the involved nuclei are currently not accessible in the laboratory and therefore theoretical models have to be invoked in order to predict reaction rates.

In astrophysical applications usually different aspects are emphasized than in pure nuclear physics investigations. Many of the latter in this long and well established field were focused on specific reactions, where all or most "ingredients" (see Sec. 3) were deduced from experiments. As long as the reaction mechanism is identified properly, this will produce highly accurate cross sections. For the majority of nuclei in astrophysical applications such information is not available. The real challenge is thus not the application of well-established models, but rather to provide all the necessary ingredients in as reliable a way as possible, also for nuclei where no such information is available.

2 Nuclear Cross Sections and Reaction Rates

The nuclear cross section σ is defined as the number of reactions ξ target^{-1} s^{-1} divided by the flux Φ of incoming particles: $\sigma = \xi/\Phi$. To compute the number of reactions r per volume and time, the velocity (energy) distribution between the interacting particles has to be considered. Nuclei in an astrophysical plasma follow a Maxwell-Boltzmann distribution (MBD) and the thermonuclear reaction rates will have the form [1]

$$\begin{aligned} r_{j,k} &= \langle \sigma v \rangle \, n_j n_k \\ \langle \sigma v \rangle : &= (\frac{8}{M\pi})^{1/2} (kT)^{-3/2} \int_0^\infty E\sigma(E) \exp(-E/kT) dE. \end{aligned} \quad (1)$$

Here M denotes the reduced mass of the target-projectile system and $n_{j,k}$ is the number of projectiles and target nuclei, respectively. In astrophysical plasmas with high densities and/or low temperatures, electron screening becomes highly important, which reduces the Coulomb repulsion.

In the laboratory, the cross section $\sigma^{0\nu}$ for targets in the ground state is usually measured. However, if the plasma is in thermal equilibrium – and this is also a prerequisite for the application of the MBD – the nuclei will rather be thermally excited [2]. This has to be accounted for by summing over the excited target states and weighting each contribution with a factor describing the probability of the thermal excitation. The ratio of the *stellar* cross section σ^* and the laboratory cross section $\sigma^{0\nu}$ is called stellar enhancement factor (SEF=$\sigma^*/\sigma^{0\nu}$). The stellar reaction rate is then obtained by inserting σ^* into Eq. (1): $r^* = \langle \sigma^* v \rangle \, n_j n_k = \langle \sigma v \rangle^* \, n_j n_k$. It should be noted that only the stellar rate r^* (involving the stellar cross section) always obeys reciprocity (because σ^* does) and that therefore only r^* can be used to compute the reverse rate. Thus, it is very important when measuring reaction cross sections in the laboratory for astrophysical application to measure the cross section for the reaction in the direction that is least affected by excited states in the target. This is almost always the exoergic reaction (i.e. $Q > 0$). Even so, the stellar rate at temperatures in excess of a few billion degrees will vary considerably from that of a determination based on targets in their ground states. The experimentally determined laboratory rate should then be multiplied by the SEF, which can, in most cases, only be determined by a theoretical calculation. Even at the low temperatures of the *s* process, the SEF can already be important. Neutron capture cross sections of isotopes in the rare earth region have recently been measured to such a high accuracy that the knowledge of precise SEFs becomes crucial for further constraining *s* process conditions [3]. In principle, sufficiently reliable SEF calculations would provide an additional thermometer for the *s*-process environment, completely independent of the usual estimates via *s*-process branchings [4].

In general, the cross section will be the sum of the cross sections resulting from compound reactions via an average over overlapping resonances (HF) and via single resonances (BW), direct reactions (DI) and interference terms:

$$\sigma(E) = \sigma^{\mathrm{HF}}(E) + \sigma^{\mathrm{BW}}(E) + \sigma^{\mathrm{DC}}(E) + \sigma^{\mathrm{int}}(E) \quad . \tag{2}$$

Depending on the number of levels per energy interval in the system projectile+target, different reaction mechanisms will dominate [5, 6]. Since different regimes of level densities are probed at the various projectile energies, the application of a specific description depends on the energy. In astrophysics, one is interested in energies in the range from a few tens of MeV down to keV or even thermal energies (depending on the charge of the projectile). For instance, when varying the energy of a neutron beam from 10 MeV down to thermal energy, the resulting cross sections will be dominated by mainly three different contributions: At the highest energy, many close resonances overlap and allow to use an average cross section calculated in the statistical model (Hauser-Feshbach, HF). To lower energies, the nuclear states become more and more widely spaced until one can identify single resonances which can be included into the HF equation as a special case, yielding the well-known Breit-Wigner (BW) shape. In between resonances the cross sections are determined by the tail of resonances and the direct (DI) contribution. At the lowest energies, the levels can be so widely spaced that the cross section is described well by the direct component alone. Extrapolations from one regime into another can be extremely misleading.

The relevant nuclear levels are found in the effective energy window of a reaction, i.e. the energy range which is mainly contributing to the determination of the nuclear

reaction rate. This energy window is usually well defined, due to the sharply peaking integrand of Eq. (1). For neutrons, it is given by the width of the peak of the MBD. For charged particles the cross section includes the penetrability through the Coulomb barrier which is exponentially increasing with increasing energy. Folding this cross section with the velocity distribution gives rise to a broader peak shifted to higher energies, the so-called Gamow peak. Using experimental information or a theoretical level density description, it is possible to determine the number of levels within the effective energy window and thus derive the applicability of the statistical model as a function of temperature [6]. Below a critical temperature, averaging over too few resonances is not appropriate anymore and the HF will misjudge the cross section. The critical temperature is especially high for targets with closed shells which exhibit widely spaced nuclear levels, and for targets close to the driplines which have low particle separation energies (and Q values).

3 The Statistical Model

The majority of nuclear reactions in astrophysics can be described in the framework of the statistical model (HF) [7]. This description assumes that the reaction proceeds via a compound nucleus which finally decays into the reaction products. With a sufficiently high level density, average cross sections

$$\sigma^{\mathrm{HF}} = \sigma_{\mathrm{form}} b_{\mathrm{dec}} = \sigma_{\mathrm{form}} \frac{\Gamma_{\mathrm{final}}}{\Gamma_{\mathrm{tot}}} \tag{3}$$

can be calculated which can be factorized into a cross section σ_{form} for the formation of the compound nucleus and a branching ratio b_{dec}, describing the probability of the decay into the channel of interest compared with the total decay probability into all possible exit channels. The partial widths Γ as well as σ_{form} are related to (averaged) transmission coefficients, which comprise the central quantities in any HF calculation.

Many nuclear properties enter the computation of the transmission coefficients: mass differences (separation energies), optical potentials, GDR widths, level densities. The transmission coefficients can be modified due to pre-equilibrium effects which are included in width fluctuation corrections [8] (see also [6] and references therein) and by isospin effects. It is in the description of the nuclear properties where the various HF models differ.

In the following sections, the most important ingredients and the usual parametrizations used in astrophysical applications are briefly discussed. A choice of what is thought of being the currently best parametrizations is incorporated in the new HF code NON-SMOKER [9], which is based on the well-known code SMOKER [10].

3.1 Optical Potentials

Early astrophysical studies (e.g. [2, 11, 12]) made use of simplified equivalent square well potentials and the black nucleus approximation. It is equivalent to a fully absorptive potential, once a particle has entered the potential well and therefore does not permit resonance effects. This leads to deviations from experimental data at low energies, especially in mass regions where broad resonances in the continuum can be populated [13]. An additional effect, which is only pronounced for α particles, is that absorption in the Coulomb barrier [14] is neglected in this approach.

Improved calculations have to employ appropriate *global* optical potentials which make use of imaginary parts describing the absorption. The situation is different for nucleon-nucleus and α-nucleus potentials. Global optical potentials are quite well defined for neutron and protons. It was shown [15, 16] that the best fit of s-wave neutron strength functions is obtained with the optical potential by [17], based on microscopic infinite nuclear matter calculations for a given density, applied with a local density approximation. It includes corrections of the imaginary part [18, 19]. A similar description can be used for protons. Numerous experimental data document the reliability of the neutron potential for astrophysical applications. For protons, data are more scarce but recent investigations [20] also show good agreement.

In the case of α-nucleus potentials, there are only few *global* parametrizations available at astrophysical energies. Most global potentials are of the Saxon–Woods form, parametrized at energies above about 70 MeV, e.g. [21, 22]. The high Coloumb barrier makes a direct experimental approach very difficult at low energies. More recently, there were attempts to extend those parametrizations to energies below 70 MeV [23]. Astrophysical calculations mostly employed a phenomenological Saxon–Woods potential based on extensive data [24]. This potential is an energy– and mass–independent mean potential. However, especially at low energies the imaginary part of the potential should be highly energy–dependent. Nevertheless, this potential proves to be very successful in describing HF cross sections. It failed so far only in one case, the recently measured ^{144}Sm(α,γ)^{148}Gd low-energy cross section [25]. Nevertheless, this showed that future improved α potentials have to take into account the mass- and energy-dependence of the potential. Several attempts have been made to construct such an improved potential. Extended investigations of α scattering data [26, 27] have shown that the data can best be described with folding potentials [28]. They also found a systematic mass- and energy-dependence. Very recently, that description was used for a global approach [9, 29]. The idea is to parametrize the data including nuclear structure information. The accuracy reached [29] is comparable to the potential of Ref. [24]. The same approach was used by [30], without including further microscopic information. However, the limitation of this method is that a Woods-Saxon term with fixed geometry is still used for the imaginary part. The resulting transmission coefficients are very sensitive to the shape of the imaginary part, which leads to an ambiguity in the parametrization. Experimental data indicate that the geometry may also be energy-dependent [23, 31, 32]. This can be understood in terms of the semi-classical theory of elastic scattering [33] which shows that with varying energy different radial parts of the potential are probed. The effect can be explicitly considered in a global potential [34]. Nevertheless, more experimental data are needed which should be consistently analyzed at different energies. Further complications arise from the fact that it is yet unclear if potentials extracted from scattering data can indeed describe transmission coefficients well [23]. Clearly, further effort has to be put into the improvement of global α-nucleus potentials at astrophysically relevant energies.

3.2 γ Width

The γ-transmission coefficients have to include the dominant E1 and M1 γ transitions. The smaller, less important M1 transitions have usually been treated with the simple single particle approach $T \propto E^3$ [35]. The E1 transitions are usually calculated on the

basis of the Lorentzian representation of the Giant Dipole Resonance (GDR). Many microscopic and macroscopic models have been devoted to the calculation of GDR energies and widths. Analytical fits as a function of mass number A and charge Z were also used in astrophysical calculations [11, 12]. An excellent fit to the GDR energies is obtained with the hydrodynamic droplet model [36]. An improved microscopic-macroscopic approach is used in most modern reaction rate calculations, based on dissipation and the coupling to quadrupole surface vibrations (see [16]).

Most recently it was shown [37] that the inclusion of pygmy resonances might have important consequences on the E1 transitions in neutron-rich nuclei far off stability. The pygmy resonances can be caused by a neutron skin which generates soft vibrational modes [38]. While the effect close to stability is small, neutron capture cross sections could be considerably enhanced close to the neutron dripline.

3.3 Level Density

Until recently, the nuclear level density (NLD) has given rise to the largest uncertainties in the description of nuclear reactions [12, 16]. For large scale astrophysical applications it is necessary to not only find reliable methods for NLD predictions but also computationally feasible ones. Such a model is the non-interacting Fermi-gas model. Most statistical model calculations use the back-shifted Fermi-gas description [39]. More sophisticated Monte Carlo shell model calculations (e.g. [40]), as well as combinatorial approaches (e.g. [41]), have shown excellent agreement with this phenomenological approach and justified the application of the Fermi-gas description. While different fits to different mass regions to obtain the free parameters were performed in many investigations [11, 12, 16], a most recent study was able to arrive at considerably improved NLDs with fewer parameters in the mass range $20 \leq A \leq 245$ [6]. They applied an energy-dependent NLD parameter [42] together with microscopic corrections from nuclear mass models. The fit to experimental NLDs is also better than a recent analytical BCS approach [43] which implemented level spacings from a microscopic mass model. (In fact, see [44, 45] for doubts on the reliability of the BCS model for neutron-rich nuclei).

Further work has to be invested in the problem of the prediction of the parity distribution at low excitation energies of the nucleus.

3.4 Isospin Effects

The original HF equation [7] implicitly assumes complete isospin mixing but can be generalized to explicitly treat the contributions of the dense background states with isospin $T^{<} = T^{\mathrm{g.s.}}$ and the isobaric analog states with $T^{>} = T^{<} + 1$ [46, 47]. The inclusion of the isospin treatment has two major effects on statistical cross section calculations in astrophysics [9]: the suppression of γ widths for reactions involving self-conjugate nuclei and the suppression of the neutron emission in proton-induced reactions. (Non-statistical effects, i.e. the appearance of isobaric analog resonances, will not be discussed here.) Firstly, in the case of (α,γ) reactions on targets with $N = Z$, the cross sections will be heavily suppressed because $T = 1$ states cannot be populated due to isospin conservation. A suppression will also be found for capture reactions leading into self-conjugate nuclei, although somewhat less pronounced because $T = 1$ states can be populated according to the isospin coupling coefficients. In previous reaction rate calculations [12, 16] the suppression of the γ–widths was treated

completely phenomenologically by employing arbitrary and mass-independent suppression factors. In the new NON-SMOKER code [9], the appropriate γ widths are automatically obtained, by explicitly accounting for $T^<$ and $T^>$ states.

Secondly, assuming incomplete isospin mixing, the strength of the neutron channel will be suppressed in comparison to the proton channel in reactions p+target [46, 48]. This leads to a smaller cross section for (p,n) reactions and an increase in the cross section of (p,γ) reactions above the neutron threshold. Such an effect has recently been found in a comparison of experimental data and NON-SMOKER results [20].

4 Direct Reactions

As stated above, the HF approach can only be applied for sufficiently high NLDs [6]. At low NLDs, the other terms in Eq. (2) will begin to dominate. Many investigations (e.g. [49, 50, 51, 52, 53, 54]) have been devoted to the calculation of direct neutron capture for light nuclei and nuclei close to magic neutron numbers. Utilizing folding potentials, these calculations can yield reliable cross sections provided that information on the bound states and the spectroscopic factors is known. Even in the regime of single resonances, the feeble DI contribution can be seen nowadays, when comparing highly precise resonance data and activation measurements (e.g. [55]).

The prediction of the DI contribution to neutron capture cross sections close to the dripline (which may be important in the r process) remains a challenge. Far off stability, the required nuclear properties are not known and have to be taken from other theories [56, 57, 58]. However, it was shown [58] that a straightforward application produces cross sections which are highly sensitive to slight changes in the predicted masses and level energies. Furthermore, it is not yet clear which spectroscopic factors to employ and how to model interference between DI and HF in a simple manner. Further work is clearly needed.

5 Summary

The new generation of HF models can make reliable predictions of nuclear cross sections. Furthermore, the applicability range of HF has been quantified and thus the boundary between different reaction mechanisms clarified. Although the phenomenological parametrizations of nuclear properties already display good quality, there is a clear need for more experimental data for checking and further improving current models. Especially investigations over a large mass range would prove useful to fill in gaps in the knowledge of the nuclear structure of many isotopes and to construct more powerful parameter systematics, which sometimes are badly known even at the line of stability. Such investigations should include neutron-, proton- and α-strength functions, as well as radiative widths, and charged particle scattering and reaction cross sections for *stable* and unstable isotopes. More capture data with self-conjugate final nuclei would also be highly desireable.

The new code NON-SMOKER [9] contains updated nuclear information as well as additional effects. The NON-SMOKER reaction rate library is electronically available at *http://quasar.physik.unibas.ch/∼tommy/reaclib.html* .

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References

[1] Fowler W.A., Caughlan G.E., & Zimmerman B.A., 1967, Ann. Rev. Astron. Astrophys. 5, 525
[2] Arnould M., 1972, A&A 19, 92
[3] Voss F., et al. , 1998, ApJ , in press; Wisshak K., et al. , this volume
[4] Käppeler F., Beer H., & Wisshak K., 1989, Rep. Prog. Phys. 52, 945
[5] Wagoner R.V., 1969, Ap. J. Suppl. 18, 247
[6] Rauscher T., Thielemann F.-K., & Kratz K.-L., 1997, Phys. Rev. C 56, 1613
[7] Hauser W., Feshbach H., 1952, Phys. Rev. 87, 366
[8] Tepel J.W., Hoffmann H.M., & Weidenmüller H.A., 1974, Phys. Lett. 49B, 1
[9] Rauscher T., Thielemann F.-K., 1998, ed Mezzacappa A., in *Stellar Evolution, Stellar Explosions, and Galactic Chemical Evolution*. IOP Publishing, Bristol, p. 519; preprint nucl-th/9802040
[10] Thielemann F.-K., Arnould M., & Truran J., 1987, ed Vangioni-Flam E., in *Advances in Nuclear Astrophysics*. Editions Frontières, Gif-sur-Yvette, p. 525
[11] Holmes J.A., et al. , 1976, ADNDT 18, 306
[12] Woosley S.E., et al. , 1978, ADNDT 22, 371
[13] Hoffman R.D., et al. , 1998, ApJ , submitted; preprint astro-ph/9809240
[14] Michaud G., Scherk L., & Vogt E., 1970, Phys. Rev. C 1, 864
[15] Thielemann F.-K., Metzinger J., & Klapdor H.V., 1983, Z. Phys. A 309, 301
[16] Cowan J.J., Thielemann F.-K., & Truran J.W., 1991, Phys. Rep. 208, 267
[17] Jeukenne J.P., Lejeune A., & Mahaux C., 1977, Phys. Rev. C 16, 80
[18] Fantoni S., Friman B.L., & Pandharipande V.R., 1981, Phys. Rev. Lett. 48, 1089
[19] Mahaux C., 1982, Phys. Rev. C 82, 1848
[20] Bork J., et al. , 1998, Phys. Rev. C 58, 524
[21] Singh P.P, Schwandt P., 1976, Nukleonika 21, 451
[22] Nolte M., Machner H., & Bojowald J., 1987, Phys. Rev. C 36, 1312
[23] Avrigeanu V., Hodgson P.E., Avrigeanu M., 1994, Phys. Rev. C 49, 2136
[24] McFadden L., Satchler G.R., 1966, Nucl. Phys. 84, 177
[25] Somorjai E., et al. , 1998, A&A 333, 1112
[26] Mohr P., et al. , 1994, eds Somorjai E., Fülöp Zs., in *Proc. Europ. Workshop on Heavy Element Nucleosynthesis*. Institute of Nuclear Research, Debrecen, p. 176
[27] Atzrott U., et al. , 1996, Phys. Rev. C 53, 1336
[28] Satchler G.R., Love W.G., 1979, Phys. Rep. 55, 183
[29] Rauscher T., 1998, eds Buballa M., et al. , in *Nuclear Astrophysics*. GSI, Darmstadt, p. 288; preprint nucl-th/9802026
[30] Grama C., Goriely S., this volume.
[31] Mohr P., et al. , 1997, Phys. Rev. C 55, 1523
[32] Budzanowski A., et al. , 1978, Phys. Rev. C 17, 951
[33] Brink D.M., Takigawa N., 1977, Nucl. Phys. A279, 159
[34] Rauscher T., 1998, ed Müller E., in *Ringberg Proceedings*. MPA, Garching, in press
[35] Blatt J.M., Weisskopf V.F., 1952, *Theoretical Nuclear Physics*. Wiley, New York
[36] Myers W.D., et al. , 1977, Phys. Rev. C 15, 2032
[37] Goriely S., 1998, Phys. Lett. B, in press; Goriely S., this volume
[38] Van Isacker P., Nagarajan M.A., & Warner D.D., 1992, Phys. Rev. C 45, R13
[39] Gilbert A., Cameron A.G.W., 1965, Can. J. Phys. 43, 1446
[40] Dean D.J., et al. , 1995, Phys. Rev. Lett. 74, 2909
[41] Paar V., Pezer R., 1997, Phys. Rev. C 55, R1637
[42] Ignatyuk A.V., Smirenkin G.N., & Tishin A.S., 1975, Yad. Fiz. 21, 485
[43] Goriely S., 1996, Nucl. Phys. A605, 28
[44] Pearson J.M., Nayak R.C., & Goriely S., 1996, Phys. Lett. B387, 455
[45] Dobaczewski J., et al. , 1996, Phys. Rev. C 53, 1
[46] Grimes S.M., et al. , 1972, Phys. Rev. C 5, 85
[47] Harney H.L., Weidenmüller H.A., & Richter A., 1977, Phys. Rev. C 16, 1774
[48] Sargood D.G., 1982, Phys. Rep. 93, 61
[49] Oberhummer H., et al. , 1996, Surv. Geophys. 17, 665
[50] Meißner J., et al. , 1996, Phys. Rev. C 53, 459/977
[51] Beer H., et al. , 1995, Phys. Rev. C 52, 3342
[52] Krausmann E., et al. , 1996, Phys. Rev. C 53, 469
[53] Mohr P., et al. , 1998, Phys. Rev. C 58, 932
[54] Mohr P., et al. , 1998, this volume
[55] Koehler P., et al. , 1998, this volume
[56] Mathews G.J., et al. , 1983, ApJ 270, 740
[57] Goriely S., 1997, A&A 325, 414
[58] Rauscher T., et al. , 1998, Phys. Rev. C 57, 2031